

From second to first order transitions in a disordered quantum magnet

L. F. Cugliandolo¹, D. R. Grempel^{2,*} and C. A. da Silva Santos³

¹ *Laboratoire de Physique Théorique de l'École Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France and Laboratoire de Physique Théorique et Hautes Énergies, Jussieu, 5ème étage, Tour 24, 4 Place Jussieu, 75005 Paris, France*

² *CEA-Service de Physique de l'État Condensé, CEA-Saclay, 91191 Gif-sur-Yvette CEDEX, France*

³ *Laboratoire de Physique Théorique et Modèles Statistiques, Bât. 100, Université Paris-Sud, Orsay, F-91405, France*
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We study the spin-glass transition in a disordered quantum model. There is a region in the phase diagram where quantum effects are small and the phase transition is second order, as in the classical case. In another region, quantum fluctuations drive the transition first order. Across the first order line the susceptibility is discontinuous and shows hysteresis. Our findings reproduce qualitatively observations on $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$. We also discuss a marginally stable spin-glass state and derive some results previously obtained from the real-time dynamics of the model coupled to a bath.

The study of quantum effects on the properties of spin glasses is a subject of great experimental and theoretical interest. Spin-glass phases have been identified in systems such as mixed hydrogen-bonded ferroelectrics [1], the dipolar magnet $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ [2,3] or Sr-doped La_2CuO_4 [4] where quantum mechanics plays a fundamental role. An important question is whether quantum spin glasses are qualitatively different from their classical counterparts at low temperature. There is growing experimental evidence that the answer to this question is affirmative both in and out of equilibrium [2]. The thermodynamics of several models of disordered magnetic systems has been investigated with various techniques. Mean-field-like models have been solved using the replica formalism in imaginary-time [5–13] and the Ising model in a transverse field has also been studied in finite dimensions [14–16]. It is generally found that, in terms of a suitably defined quantum parameter Γ , a boundary $\Gamma_c(T)$ in the $\Gamma - T$ plane separates spin-glass (SG) and paramagnetic (PM) phases. The transition line ends at a quantum critical point at $T = 0$, $\Gamma_c(0)$ above which the system is paramagnetic at all temperatures. In the case of the quantum spherical p -spin model, the real-time dynamics of the system coupled to a phonon bath was also investigated [17]. In this case, a boundary $\Gamma_d(T)$ was found across which there is a *dynamic* phase transition from a PM state with equilibrium dynamics to a SG with non-stationary, aging, dynamics.

In this paper we investigate in detail the equilibrium properties of this model. We find that a tricritical point (T^*, Γ^*) divides the line $\Gamma_c(T)$ in two parts. For $T \geq T^*$, the SG transition is of second order and the behavior of the quantum system is qualitatively similar to that of the classical one. However, for $T < T^*$ quantum fluctuations drive the transition first order. The magnetic susceptibility is discontinuous and shows hysteresis across the first-order line. These findings reproduce qualitatively the observed behavior of $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ in a transverse magnetic field [2,3]. The equations describing this system are non-linear and there is multiplicity of solutions in parts of the phase diagram. We found as a surprise that

the usual criteria used to choose between them have to be reinterpreted in order to get physically meaningful solutions in the region $T < T^*$. We also discuss the properties of solutions obtained through the use of the *marginality condition*, an approach recently applied to the study of quantum problems [10,18]. It is known from work on classical models [19] that the results of this approach are closely related to those obtained from the analysis of the real-time dynamics of the system. We explicitly show that this holds true in our quantum case. This enables us to identify the dynamical transition line $\Gamma_d(T)$ and to derive certain properties of the non-equilibrium dynamics using the replica calculation.

The Hamiltonian of the quantum p -spin spherical model is

$$H[\mathbf{P}, \mathbf{s}, J] = \frac{1}{2M} \sum_{i=1}^N P_i^2 - \sum_{i_1 < \dots < i_p}^N J_{i_1 \dots i_p} s_{i_1} \dots s_{i_p}, \quad (1)$$

where s_i is a scalar spin variable and the conjugated momenta P_i satisfy the commutation relations $[P_i, s_j] = -i\hbar\delta_{ij}$. A Lagrange multiplier z enforces the spherical constraint $1/N \sum_{i=1}^N \langle s_i^2 \rangle = 1$. The interactions $J_{i_1 \dots i_p}$ are chosen from a Gaussian distribution with zero mean and variance $[J_{i_1 \dots i_p}^2]_J = \tilde{J}^2 p! / (2N^{p-1})$. The model has glassy properties for all $p \geq 2$. The Hamiltonian (1) may be interpreted in several ways. It represents a non-linear generalization of the quantum-rotor spin-glass models discussed in the literature [12]. It also describes a quantum particle moving in an N (eventually infinite) dimensional space in the presence of a random potential. Finally, its partition function is formally identical to that of a classical chain of “length” $L = \beta\hbar$ embedded in an N -dimensional random environment.

The equilibrium properties of the model are obtained using a replicated imaginary-time path integral formalism [5]. In the large N limit, the saddle-point evaluation of the partition-function allows us to define the order-parameter $Q_{ab}(\tau - \tau') = 1/N \sum_{i=1}^N \langle T s_i^a(\tau) s_i^b(\tau') \rangle$ where $a, b = 1, \dots, n$ denote the replica indices and T the imaginary-time ordering operator. In terms of Q_{ab}

the free-energy per spin reads

$$F = \lim_{n \rightarrow 0} \frac{1}{2n} \left\{ -\frac{1}{\beta} \sum_{\omega_k} \left[\text{Tr} \ln \left(\frac{\tilde{Q}(\omega_k)}{\beta \hbar} \right) - n ((M\omega_k^2 + z) \times \frac{\tilde{q}_d(\omega_k)}{\hbar} - 1) \right] - nz - \frac{\tilde{J}^2}{2\hbar} \sum_{ab} \int_0^{\beta \hbar} d\tau Q_{ab}^p(\tau) \right\} \quad (2)$$

where $\beta = 1/(k_B T)$ is the inverse temperature, $\omega_k = 2\pi k/\beta$ are the Matsubara frequencies, $\tilde{Q}_{ab}(\omega_k) = \int_0^{\beta \hbar} d\tau Q_{ab}(\tau) e^{i\omega_k \tau}$ and $\tilde{q}_d(\omega_k) = \tilde{Q}_{aa}(\omega_k)$. From here on we take \tilde{J} as the unit of energy, \hbar/\tilde{J} as the unit of time, and work with dimensionless quantities. Quantum fluctuations are controlled by the parameter $\Gamma \equiv \hbar^2/(\tilde{J}M)$. The classical limit of the model [20] is recovered when $\Gamma \rightarrow 0$. The equilibrium solutions are determined by requiring that $\tilde{Q}_{ab}(\omega_k)$, parametrized according to different *ansatze*, be an extremum of F . In the following we concentrate on the case $p \geq 3$. The phenomenology of the $p = 2$ case [12,13] is not as rich.

For sufficiently high T and/or Γ , thermal and/or quantum fluctuations destroy the SG phase and the system is in the PM phase. The free-energy is then extremal for $Q_{ab}(\tau) = \delta_{ab} q_d(\tau)$. Its Fourier transform is the solution of the equation

$$\tilde{q}_d(\omega_k) = [\omega_k^2/\Gamma + z - \Sigma(\omega_k)]^{-1}, \quad (3)$$

with $\Sigma(\omega_k) = p/2 \int_0^{\beta} d\tau q_d^{p-1}(\tau) e^{i\omega_k \tau}$ and z is determined from $q_d(0) = 1$. The above equation is non-linear and may have several solutions, some of which may be spurious. We solved Eq. (3) numerically for $p = 3$. We found that for $T > T^* \approx 1/6$ there is only one solution, irrespective of the value of Γ . However, for $T < T^*$, three solutions coexist in a finite region of the $T - \Gamma$ plane (not including the $\Gamma=0$ axis). One of them is unstable and can be discarded from the start. We discuss below how to choose the physical solution between the remaining two. In the SG phase, inspired by the classical case [20], we searched for one-step RSB solutions of the form $Q_{ab}(\tau) = q'_d(\tau)\delta_{ab} + q_{EA}\epsilon_{ab}$, where $\epsilon_{ab} = 1$ if a and b belong to the same diagonal block of size $m \times m$ and zero otherwise, and $q'_d(\tau) = q_d(\tau) - q_{EA}$. The diagonal part, $q_d(\tau)$, the breaking point, m , and the Edwards-Anderson order parameter, q_{EA} , are determined by extremizing F . We find

$$\tilde{q}'_d(\omega_k) = [\omega_k^2/\Gamma + z' - (\Sigma'(\omega_k) - \Sigma'(0))]^{-1}, \quad (4)$$

where $\Sigma'(\tau) = p/2(q^{p-1}(\tau) - q_{EA}^{p-1})$, $z' = p/2\beta m q_{EA}^{p-1}(1 + x_p)/x_p$ and

$$m = T x_p \sqrt{2/(p(1 + x_p))} q_{EA}^{-p/2}. \quad (5)$$

The parameter x_p , solution of an algebraic equation, depends on p only, and we found $x_3 = 1.817$. The condition $q_d(0) = 1$ now yields an equation for the breaking point of the form $m \equiv \mu_T(\Gamma)$. Solutions of Eq. (4)

exist only for $\Gamma \leq \Gamma_{\max}(T)$. Above this value, quantum fluctuations destroy the SG phase. We found that the function $\mu_T(\Gamma)$ has two real branches in the interval $0 \leq \Gamma \leq \Gamma_{\max}(T)$. The physical values of m are on the lowest branch which verifies $\mu_T(0) = m_{\text{class}}(T)$, the classical breaking point parameter. The situations above and below T^* are different. For $T \geq T^*$ (but lower than the classical transition temperature), $m_{\max} \equiv m(\Gamma_{\max}) = 1$, its largest possible value. For $T < T^*$, instead, $m_{\max} < 1$. In both cases, q_{EA} is finite at $\Gamma_{\max}(T)$. We discuss below the consequences of these facts. We found that $\lim_{T \rightarrow 0} m_{\max}(T) = 0$, implying that replica symmetry is restored at the quantum critical point as in the model discussed in reference [10]. All these conclusions, obtained from the numerical analysis of the $p = 3$ case, also follow from an approximate analytical solution of the equations for arbitrary $p \geq 3$ [21].

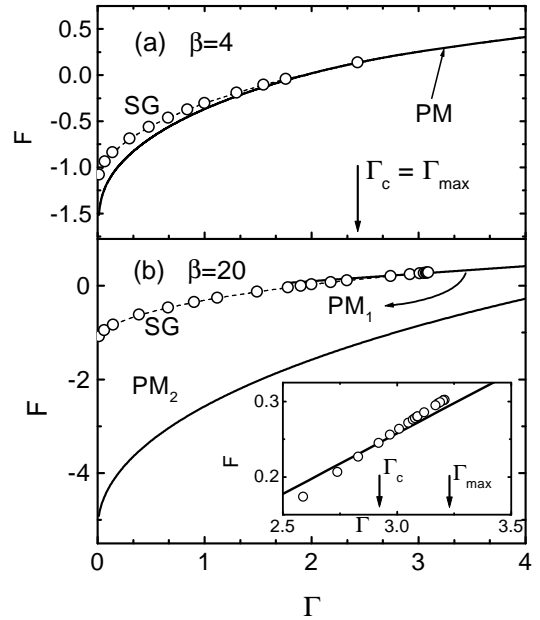


FIG. 1. Free-energies of the different PM (solid lines) and SG (symbols) phases above (a) and below (b) T^* . The inset in panel (b) shows in detail the crossing of the free-energies at the critical point for $T < T^*$.

PM solutions exist throughout the $T - \Gamma$ plane. The free-energies of the different states must thus be compared in order to construct a phase diagram. Figs. 1(a) and (b) show the Γ -dependence of the PM and SG free-energies for the case $p = 3$ computed from Eq. (2) for two temperatures, above and below T^* . Solid lines and symbols represent the PM and SG solutions, respectively. The curves end at the point where the corresponding solution disappears. It may be seen that for $T > T^*$ the free-energies of the two states intersect precisely at $\Gamma_c(T) = \Gamma_{\max}(T)$: the SG solution does not extend beyond the transition point and no hysteresis is expected. Below the critical point, $F_{\text{SG}} > F_{\text{PM}}$ meaning that the

SG solution *maximizes* the free-energy. This is the usual situation encountered in replica theories of classical spin glasses. As in the classical case, q_{EA} is *discontinuous* at the transition. The latter is nevertheless of *second* order because $m = 1$ at Γ_c and, therefore, the effective number of degrees of freedom participating in the transition $(1 - m)q_{\text{EA}} \rightarrow 0$ at Γ_c . There is no latent heat and the linear susceptibility is continuous.

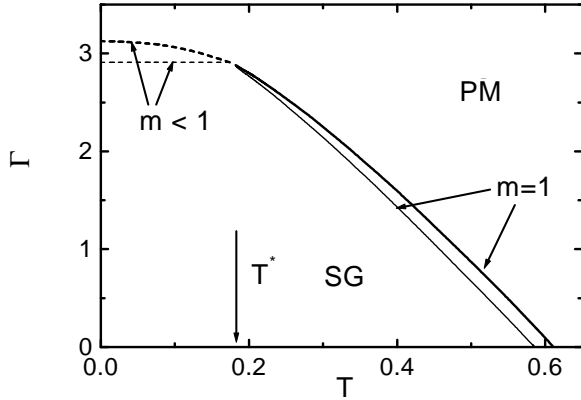


FIG. 2. Static (thin lines) and dynamic (thick lines) phase diagrams of the p -spin model for $p = 3$. Solid and dashed lines represent second and first order transitions, respectively.

The situation is more involved below T^* . To start with, one has to choose between the two PM solutions labeled PM_1 and PM_2 in Fig. 1. Naively, one would choose the solution with the lowest free-energy, *i.e.*, PM_2 . However, this solution has unphysical properties. As shown in Fig. 1(b), its free-energy *never* intersects that of the SG phase. Both the free-energy and the susceptibility diverge as $T \rightarrow 0$. Furthermore, this solution disappears at a finite value of Γ (not shown in the figure) and cannot thus be reached starting from $\Gamma = \infty$. On the other hand, it is clear that the ground-state of Hamiltonian (1) must have finite susceptibility and energy. We thus conclude that PM_2 is a spurious solution and that PM_1 has to be chosen even if its free-energy is *higher* [22]. The free-energies of the SG and PM_1 states cross at $\Gamma_c < \Gamma_{\text{max}}$ as shown in the inset in Fig. 1(b). In the low temperature phase, $F_{\text{SG}} < F_{\text{PM}}$, the opposite of what we found for $T > T^*$. The SG and PM solutions extend beyond the point where they cross. There is a region of phase co-existence and hysteresis effects are thus expected in the behavior of observables.

Since now q_{EA} and m are discontinuous at Γ_c the thermodynamic transition is *first* order with latent heat and discontinuous susceptibility (see below). The phase diagram resulting from this analysis is represented in Fig. 2 (thin lines). The flat section is the first-order line. We have computed the Edwards-Anderson order parameter and the susceptibility, $\chi = \int_0^\beta d\tau [q_d(\tau) - (1 - m)q_{\text{EA}}]$, as functions of Γ for the $p = 3$ model. The results are displayed in Fig. 3. The susceptibility has a cusp at Γ_c

for $T > T^*$ and a discontinuity for $T < T^*$. The dotted lines correspond to the regions of metastability. Their end points give the amplitude of the ideal hysteresis cycle. The importance of quantum fluctuations may be appreciated from the fact that half way from the transition the order parameter is already reduced by a factor of two. It can be shown analytically [21] that the spectrum of magnetic excitations at $T = 0$ is gaped *both* in the PM and SG phases for all $\Gamma \neq 0$ (see below, however). Consequently, the latent heat vanishes exponentially as $T \rightarrow 0$. Since it also vanishes at T^* , it must have a maximum at some intermediate temperature.

First order quantum transitions were also found in two other models, the fermionic SK-like spin-glass model [9] and a p -spin model in a transverse field [11]. In contrast, the SG transitions of the Heisenberg EA model and of the SK model in a transverse field are known to be second order [8]. This is also true in finite dimensions [14–16]. Early experiments on $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ gave some indications that the second order SG transition seen above 25 mK, might become first order at lower temperatures [2]. More recently, hysteresis effects have been observed in this system as a function of the transverse field [3], giving further support to this idea. The model that we study here captures this phenomenology.

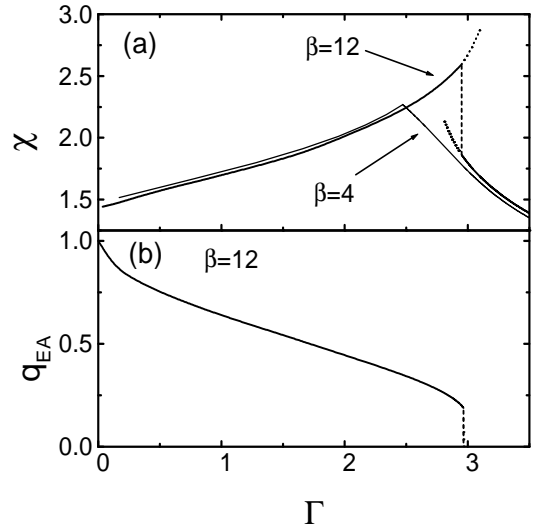


FIG. 3. Magnetic susceptibility (a) and Edwards-Anderson order parameter (b) of the $p=3$ model.

We discuss next the consequences of the use of the marginality condition [19] rather than thermodynamics in the determination of the breaking point. In this approach it is not required that F be an extremum with respect to m but that the SG phase be marginally stable. This implies that the “replicon” eigenvalue Λ must vanish throughout the low-temperature phase. The calculation of Λ [21] is analogous to the classical one [20]. The result is

$$\Lambda = \left[\frac{\tilde{q}_d(0) + \beta q_{\text{EA}}(m-1)}{\tilde{q}_d^2(0) - \beta^2 q_{\text{EA}}^2(m-1) + \tilde{q}_d(0)\beta q_{\text{EA}}(m-2)} \right]^2 \beta^2 - \frac{\beta^2}{2} p(p-1) q_{\text{EA}}^{p-2}. \quad (6)$$

The value of m follows from the equation $\Lambda = 0$, that combined with the equation $\delta F/\delta q_{\text{EA}} = 0$, yields

$$m = T(p-2)\sqrt{2/(p(p-1))} q_{\text{EA}}^{-p/2}. \quad (7)$$

Notice that this expression is equivalent to Eq.(5) with the substitution $x_p \rightarrow (p-2)$. Interestingly enough, Eq.(7) is identical to the equation found for the fluctuation-dissipation theorem (FDT) violation parameter, X , in the real-time dynamical calculation [17]. Moreover, the static and dynamical equations for q_{EA} are also identical which implies that $m = X$. The coincidence between the values of X and m for the marginal SG state has been noticed several times for classical models. This is the first explicit evidence of its validity in a quantum problem. X is related to the effective temperature [23] of the system, $T_{\text{eff}} = X^{-1}T$, where T is the temperature of the thermal bath it is in contact with. Values of $X \neq 1$ signal the presence of a non-stationary dynamics and of FDT violations. The fact that $\beta X = \beta m \rightarrow \text{const}$ when $T \rightarrow 0$ shows that a non-trivial T_{eff} is generated even when the temperature of the bath vanishes. We have also shown analytically [21] that the internal energy, computed from $U = \partial(\beta F)/\partial\beta$ at *constant* m , coincides with the long-time limit of the energy per spin as obtained from dynamics [17]. The dynamic transition line $\Gamma_d(T)$ may be thus identified as the boundary of the region in the T - Γ plane where the marginally stable SG exists. Below this line, the dynamics of the system becomes non-stationary and FDT violations set in. The dynamic phase diagram for $p = 3$ is shown in Fig.2 (thick lines). As in the equilibrium case, m is discontinuous across the dashed line. Γ_d lies always above Γ_c suggesting that the equilibrium state can never be reached dynamically starting from an initial state in the PM phase. The two lines are extremely close to each other for $T \sim T^*$. Within the accuracy of our calculations we cannot assert whether they precisely touch at T^* , an intriguing possibility. In the region $T < T^*$, m varies continuously along $\Gamma_d(T)$ and vanishes at the quantum critical point. This has a consequence of potential interest for experiment: FDT violations are predicted to appear suddenly rather than gradually as Γ_d is crossed coming from the high Γ region for $T < T^*$. The stationary part of the time-dependent susceptibility in the SG phase can be calculated by analytic continuation of $\tilde{q}'_d(\omega_k)$. It may be shown that the excitation spectrum of the marginal SG state is gapless [21]. Furthermore, $\chi''(\omega)$ may be calculated exactly for $T, \omega \rightarrow 0$. The result is

$$\lim_{\omega \rightarrow 0} \frac{\chi''(\omega)}{\omega} = \frac{1}{\Gamma} \left[\frac{2q_{\text{EA}}^{(2-p)}}{p(p-1)} \right]^{3/4}. \quad (8)$$

A linear excitation spectrum has also been found in the case of the Heisenberg spin glass model [10]. However, a gapless spectrum is not a consequence of Goldstone's theorem here as our model does not have any continuous symmetry. A more extended discussion of our results will be presented in a forthcoming paper [21].

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* On leave from CEA-Grenoble, SPSMS, F-38054 Grenoble Cedex 9, France.

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